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Coherent Rotation and Effective Anisotropy

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It is shown in this paper that the concept of effective anisotropy is of sound physical sense only when the nucleation mode is coherent rotation. Comparison of coherent and incoherent nucleation fields demonstrates that the coherent rotation can take place at very small defect size. The critical size below which the coherent rotation is favorable is roughly the domain wall-width with 3-D soft defects and is smaller for oriented exchange-coupled permanent magnets with planar soft defects. The effect of misaligned grains has also been considered and it is illustrated that the effective anisotropy has to be used very carefully: it can only be used in limited cases and its expression varies as the microstructures change.

Index Terms—Coherent rotation, effective anisotropy, nucleation modes.

I. INTRODUCTION

THE THEORETICAL understanding of the nucleation modes for magnetic systems can be dated back to the late 1940s, when Stoner and Wohlfarth proposed a theory based on the coherent rotation of the magnetic moments with respect to their easy axis [1], [2]. It is clear only after the development of the micromagnetics in the 1960s by Brown and Aharoni etc. [3]–[6], [15] that the Stoner and Wohlfarth (SW) coherent rotation is only one of possible nucleation modes. Nonuniform modes, such as curling, buckling and twisting, were discovered later [4]–[6]. A frequently overlooked aspect of the problem is that the nucleation modes have to be obtained by comparing the nucleation fields (the real mode corresponds to the smallest nucleation field) for exchange-coupled systems [4]–[7]. In particular, an “effective anisotropy” has been used to calculate the coercivity, which in some cases explains the experimental coercivity quite well [8]–[11]. In this work, nucleation modes will be derived from reliable micromagnetic calculation. The validity of the effective anisotropy and its restriction will be discussed.

II. COHERENT ROTATION ISOLATED AND COUPLED MATERIALS

Consider first one isolated crystallite having an intrinsic saturation magnetization M_S , whose easy magnetic axis oriented at an angle α to the direction of the applied field H . The equilibrium angle θ between the magnetization and the applied field is that which minimizes the total energy density

$$\gamma = K \sin^2(\theta - \alpha) - M_S H \cos \theta. \quad (1)$$

Setting $\partial\gamma/\partial\theta = 0$ and $\partial^2\gamma/\partial\theta^2 > 0$, we obtain the hysteresis loops and coercivity for arbitrary α . In particular, when the easy axis is parallel to the applied field, $\alpha = 0$, the coercivity and nucleation field are given by $H_c = H_N = H_K$, where the anisotropy field $H_K = 2K/M_S$. This nucleation mode, $\theta \equiv 0$ before the nucleation and $\theta \equiv \pi$ after the nucleation, as pointed

out by Brown [3]–[5], [15] is the simplest mode, i.e., coherent rotation. The corresponding hysteresis loop is rectangular.

The calculated coercivity is much larger than the observed experimental one. This discrepancy is called as Brown’s paradox [3]–[6], [15], which is due mainly to the crystalline defects and the intergrain interaction, especially the exchange interaction. The nucleation modes have been obtained for the exchange-coupled composite materials with both hard and soft phases. We start with the coherent rotation mode. For simplicity the easy axes of the hard and soft phases are both assumed to be in the applied field direction. The total energy density is

$$\gamma = f^h(K^h \sin^2 \theta - M_S^h H \cos \theta) + f^s(K^s \sin^2 \theta - M_S^s H \cos \theta) \quad (2)$$

where f is the volume fraction and the superscripts h and s denote the hard and soft phases respectively. This equation is the same as (1) except that the anisotropy K and the magnetization M_S in (1) are replaced by

$$K^{\text{eff}} = f^h K^h + f^s K^s \quad (3)$$

$$M_S^{\text{eff}} = f^h M_S^h + f^s M_S^s. \quad (4)$$

Here the effective anisotropy has been introduced, which is basically the average anisotropy of the hard and soft phases [8]–[11]. The hysteresis loop given by the minimization of (2) is rectangular, with the switch field given by

$$H_c = 2(f^h K^h + f^s K^s)/(f^s M_S^s + f^h M_S^h). \quad (5)$$

This formula gives the nucleation field and coercivity of the fully exchange-coupled two-phase materials. Similar results have been given by [8] based on some sort of perturbation theory.

III. COMPARISON OF INCOHERENT AND COHERENT MODES IN COMPOSITE MATERIALS

The incoherent mode has been calculated in [7], [8], [12], and [13] for an exchange-coupled hard/soft/hard system. The results could be extended to a multilayer with the hard and soft layers

arranged alternatively. In this case the total magnetic energy per unit area can be expressed as

$$\gamma = \int_0^{L^h} \left[A^h \left[\frac{d\theta}{dz} \right]^2 + K^h \sin^2 \theta - M_S^h H \cos \theta \right] dz + \int_{-L^s/2}^0 \left[A^s \left[\frac{d\theta}{dz} \right]^2 + K^s \sin^2 \theta - M_S^s H \cos \theta \right] dz \quad (6)$$

where A is the exchange energy constant and L is the thickness of the layer. By applying the variational method to (6) with suitable boundary conditions [7], [13], we obtain the nucleation field as well as the nucleation modes.

At the nucleation point, the deviation of the angle θ from the saturation state is small. Thus, the nucleation field can be derived based on the series expansion, which is

$$\frac{\pi L^s}{2\Delta^s} = \tan^{-1} \frac{\sqrt{A^h K^h (1 + h_N^h)}}{\sqrt{A^s K^s (-1 - h_N^s)}} / \sqrt{-1 - h_N^s} \quad (7)$$

with the angular distribution in the soft and hard phases given by where the reduced applied field $h = H/H_K$ and $h_N = -H_N/H_K$ are introduced. $\Delta = \pi\sqrt{A/K}$ is the Bloch wall width. θ^θ and θ^s are the directions of magnetization at the interface ($z = 0$) and at the center of the soft layer ($z = -L^s/2$). The mode according to (8) and (9), shown at the bottom of the page, is apparently an incoherent mode and the nucleation for both the hard and soft phases occurs simultaneously. One can check that the coherent mode, i.e., $\theta \equiv 0$ before the nucleation and $\theta \equiv \pi$ after the nucleation also minimizes the energy given by (6). Substituting $f^s = L^s/(L^s + L^h)$ and $f^h = 1 - f^s$ into (5) we have the nucleation field for the coherent mode as

$$H_c = 2(L^h K^h + L^s K^s)/(L^s M_S^s + L^h M_S^h). \quad (10)$$

Fig. 1 shows the calculated nucleation fields based on (7) and (10) for an $\text{Nd}_2\text{Fe}_{14}\text{B}/\alpha\text{-Fe}/\text{Nd}_2\text{Fe}_{14}\text{B}$ trilayer as a function of the soft layer thickness L^s . The material parameters are listed in Table I.

As L^s increases from 0 to infinity, H_N of both the coherent and incoherent modes decreases smoothly from H_K^h to H_K^s . The coherent nucleation field at small L^s goes down with L^s linearly, whereas the drop of the incoherent nucleation field with L^s is much faster in this region. For very thin soft layer, (7) reduces to $H_N/H_K^h = 1 - [(\pi L^s/2\Delta^h)(M_S^s/M_S^h)]^2$ [7]. H_N falls with L^s parabolically rather than linearly. Thus the coherent nucleation field is smaller only for very small L^s . Further, while the coherent H_N increases with L^h , the incoherent H_N is independent of L^h . Thus the critical thickness below which the

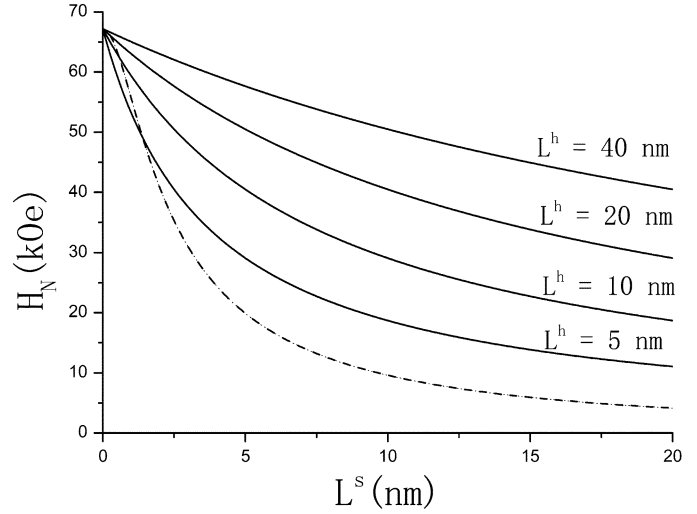


Fig. 1. Comparison of coherent (solid lines) and incoherent (dashed line) nucleation fields for a $\text{Nd}_2\text{Fe}_{14}\text{B}/\text{Fe}/\text{Nd}_2\text{Fe}_{14}\text{B}$ trilayer system as a function of the soft layer thickness.

coherent mode is favorable decreases with L^h . For $L^h = 40$ nm, the critical thickness is rather small (less than 0.2 nm). Calculation of other hard/soft multilayers shows similar results. A soft layer can be regarded as a planar soft defect, which is normally present in “single-phase” hard magnetic materials with large L^h . Thus in such materials, the coherent rotation is an unfavorable nucleation mode with larger H_N and the effective anisotropy is physically invalid.

The incoherent H_N has also been calculated for a spherical soft inclusion in a hard magnetic matrix based on a method by [8]

$$\begin{aligned} \frac{A^s}{A^h} \left[\frac{D}{2} \sqrt{\frac{M_S^s H_N - 2K^s}{2A^s}} \right. \\ \left. \times \cot \left(\frac{D}{2} \sqrt{\frac{M_S^s H_N - 2K^s}{2A^s}} \right) - 1 \right] \\ + 1 + \frac{D}{2} \sqrt{\frac{2K^h - M_S^h H_N}{2A^h}} = 0 \end{aligned} \quad (11)$$

where D is the diameter of the soft inclusion. The reliability of (11) can be easily checked. For example, taking K^s in (11) as 0, we obtain (5) of [8].

In this case the coherent nucleation field is still given by (5). Here $f^s = \pi D^3/(6a^3)$ and a is the size of the hard magnetic matrix. Fig. 2 shows the calculated coherent and incoherent nucleation fields for $\text{Nd}_2\text{Fe}_{14}\text{B}$ with $\alpha\text{-Fe}$ as the soft inclusion. The coherent mode generally has larger nucleation field than the incoherent mode and thus it is the unfavorable nucleation mode.

$$\theta/\theta^s = \cos[\pi\sqrt{-1 - h^s}(z + L)/\Delta^s] \quad (8)$$

$$\sqrt{1 + h^h} \frac{\pi z}{\Delta^h} = \ln \frac{\tan(\theta/2)[\sqrt{-1/h^h - 1} + \sqrt{-1/h^h - 1 - \tan^2(\theta^0/2)}]}{\tan(\theta^0/2)[\sqrt{-1/h^h - 1} + \sqrt{-1/h^h - 1 - \tan^2(\theta/2)}]} \quad (9)$$

TABLE I
MAGNETIC PROPERTIES FOR VARIOUS MAGNETIC MATERIALS

Material	M_S (kG)	K ($\times 10^7$ erg/cm ³)	A ($\times 10^{-7}$ erg/cm)	Δ (nm)	H_K (kOe)
Nd ₂ Fe ₁₄ B	1.28	4.3	7.7	4.2	67.2
Sm ₂ Fe ₁₇ N ₃	1.23	12.	10.7	3.0	195.
SmCo ₅	0.84	17.1	12.	2.6	407.
α -Fe	1.71	0.046	25.	73.2	0.54

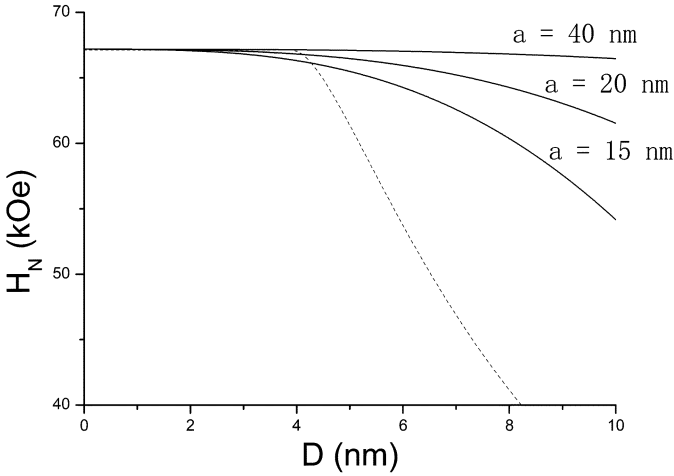


Fig. 2. Nucleation fields as a function of D , the diameter of the α -Fe inclusion in a Nd₂Fe₁₄B matrix. The solid lines show coherent nucleation field for various matrix size a while the dashed line denotes the incoherent nucleation field.

However, the incoherent nucleation field can be found only for large soft inclusions. For small D , (11) does not work [(11) has no solution for small D] and the coherent rotation is the only possible nucleation mode. The critical size is roughly the Bloch wall of the hard phase, i.e., 4.3 nm for Nd₂Fe₁₄B (see Table I).

From the above discussion it can be seen that the coherent mode can only happen in materials composed of small grains where the exchange coupling dominates over the anisotropy energy. For larger grains, non-coherent nucleation mode dominates and the concept of effective anisotropy has no physical meaning, where H_N deviates significantly from (5).

IV. PERPENDICULAR EASY AXIS

In the previous sections the magnets are assumed to be perfectly oriented materials and the calculated coherent nucleation field is much larger than the experimental coercivity. In reality, most magnets have some sort of easy axis distribution. To investigate the effect of misaligned grains let's assume that the easy axes of the soft grain are perpendicular to the applied field. Substituting K^s with $-K^s$ in (3) and (5), we have

$$K^{\text{eff}} = f^h K^h - f^s K^s \quad (12)$$

$$H_c = 2(f^h K^h - f^s K^s) / (f^h M_S^h + f^s M_S^s). \quad (13)$$

Here the effective anisotropy and nucleation field of the coherent mode decreases rather than increases with the anisotropy of the

soft phase. In particular, taking $K^s = K^h$, we have both K^{eff} and H_N as 0, which explains the very small coercivity in some single-phase permanent magnets. The corresponding hysteresis loop is also rectangular.

The incoherent nucleation field in such a case can be obtained similarly. Substituting K^s with $-K^s$ in (7), we have

$$\frac{\pi L^s}{2\Delta^s} = \tan^{-1} \frac{\sqrt{A^h K^h (1 + h_N^h)}}{\sqrt{A^s K^s (1 - h_N^s)}} / \sqrt{1 - h_N^s}. \quad (14)$$

Similar result has been obtained by Hu and Kawazoe for exchange-coupled double layers [14, eq. (25)]. A close inspection of (13) shows that the positive nucleation field can be obtained only for large L^s . The critical thickness below which the negative nucleation field takes place varies with the material parameters. In the case of single-phased permanent magnets, $K^s = K^h$, the critical thickness L_{crit} is $\Delta/2$. This critical thickness is the same as the thickness below which the coherent nucleation mode takes place. L_{crit} is rather small for rare-earth iron and rare-earth cobalt materials (see Table I), indicating that the coherent rotation can seldom take place in these novel magnets and the effective anisotropy should be used carefully.

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